A Note on Regularized Shannon's Sampling Formulae

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Error estimation is given for a regularized Shannon's sampling formulae, which was found to be accurate and robust for numerically solving partial differential equations.

Key words. Shannon's sampling formulae, error estimate, regularization.

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I. INTRODUCTION

In previous work [1], one of the present authors proposed a discrete singular convolution (DSC) algorithm for computer realization of singular convolutions involving singular kernels of delta type, Abel type and Hilbert type. One of illustrations for the algorithm was Shannon's sampling formulae [2] which plays an important role in the approximation of the delta distribution and generalized derivatives [3]. However, in practical computations, the truncation error of Shannon's sampling formulae is substantial [4]. A regularization technique [5] was used to construct a regularized Shannon's sampling formulae [1,6], which was found to be extremely accurate and robust for resolving various challenging dynamical problems, such as the homoclinic orbit excitation of the Sine-Gordon equation [7], the Navier-Stokes flow in complex geometries [8], shock capturing of the inviscid Burgers' equation [9], molecular quantum system described by the Schrödinger equation [10] and nonlinear pattern formation of the Cahn-Hilliard equation [11].

The objective of the present note is to provide a theoretical analysis for the previous excellent numerical results. Rigorous error estimations of the regularized Shannon's sampling formulae are given for their applications to interpolations and derivatives of a function.

II. MAIN RESULT

Theorem. Let f be a function $f \in L^2(R) \cap C^s(R)$ and bandlimited to B, ($B < \frac{\pi}{\Delta}$, Δ is the grid spacing). For a fixed $t \in R$ and $\sigma > 0$, denote $g(x) = f(x)H_k(\frac{t-x}{\sqrt{2}\sigma})$, where $H_k(x)$ is the kth order Hermite polynomial. If $g(x)$ satisfies

$$g'(x) \le g(x)\frac{(x-t)}{\sigma^2} \tag{1}$$

for $x \ge t + (M_1 - 1)\Delta$, and

$$g'(x) \ge g(x)\frac{(x-t)}{\sigma^2} \tag{2}$$

for $x \le t - M_2\Delta$, where $M_1, M_2 \in \mathcal{N}$, then for any $s \in \mathcal{Z}^+$

$$
\left\| f^{(s)}(t) - \sum_{n=\lceil \frac{t}{\Delta}\rceil - M_2}^{\lceil \frac{t}{\Delta}\rceil + M_1} f(n\Delta)\left[\frac{\sin\frac{\pi}{\Delta}(t-n\Delta)}{\frac{\pi}{\Delta}(t-n\Delta)}\exp(-\frac{(t-n\Delta)^2}{2\sigma^2})\right]^{(s)} \right\|_{L^2(R)}
$$

$$
\le \sqrt{3}\left[\frac{\|f^{(s)}(t)\|_{L^2(R)}}{2\pi\sigma(\frac{\pi}{\Delta}-B)\exp(\frac{\sigma^2(\frac{\pi}{\Delta}-B)^2}{2})} \right.
$$

$$
+ \frac{\|f(t)\|_{L^2(R)}\sum_{i+j+k=s}\frac{s!\pi^{i-1}H_k(\frac{-M_1\Delta}{\sqrt{2}\sigma})}{i!k!\Delta^{i-1}(\sqrt{2}\sigma)^k((M_1-1)\Delta)^{j+1}}}{\exp(\frac{(M_1\Delta)^2}{2\sigma^2})}
$$

$$
\left. + \frac{\|f(t)\|_{L^2(R)}\sum_{i+j+k=s}\frac{s!\pi^{i-1}H_k(\frac{-M_2\Delta}{\sqrt{2}\sigma})}{i!k!\Delta^{i-1}(\sqrt{2}\sigma)^k(M_2\Delta)^{j+1}}}{\exp(\frac{(M_2\Delta)^2}{2\sigma^2})} \right], \tag{3}
$$

where superscript, (s), denotes the sth order derivative.

III. PROOF

A. Separation of the error

The error breaks naturally into a few components. Denote

$$E(t) = f^{(s)}(t) - \sum_{n=\lceil \frac{t}{\Delta} \rceil - M_2}^{n=\lceil \frac{t}{\Delta} \rceil + M_1} f(n\Delta) \left[\frac{\sin\left(\frac{\pi}{\Delta}(t - n\Delta)\right)}{\frac{\pi}{\Delta}(t - n\Delta)} \exp\left(-\frac{(t - n\Delta)^2}{2\sigma^2}\right) \right]^{(s)} \tag{4}$$

$$E_1(t) = \sum_{n=-\infty}^{n=+\infty} f(n\Delta) \left[\frac{\sin\left(\frac{\pi}{\Delta}(t - n\Delta)\right)}{\frac{\pi}{\Delta}(t - n\Delta)} - \frac{\sin\left(\frac{\pi}{\Delta}(t - n\Delta)\right)}{\frac{\pi}{\Delta}(t - n\Delta)} \exp\left(-\frac{(t - n\Delta)^2}{2\sigma^2}\right) \right]^{(s)} \tag{5}$$

$$E_2(t) = \sum_{n \geq \lceil \frac{t}{\Delta} \rceil + M_1} f(n\Delta) \left[\frac{\sin\left(\frac{\pi}{\Delta}(t - n\Delta)\right)}{\frac{\pi}{\Delta}(t - n\Delta)} \exp\left(-\frac{(t - n\Delta)^2}{2\sigma^2}\right) \right]^{(s)} \tag{6}$$

$$E_3(t) = \sum_{n \leq \lceil \frac{t}{\Delta} \rceil - M_2} f(n\Delta) \left[\frac{\sin\left(\frac{\pi}{\Delta}(t - n\Delta)\right)}{\frac{\pi}{\Delta}(t - n\Delta)} \exp\left(-\frac{(t - n\Delta)^2}{2\sigma^2}\right) \right]^{(s)}. \tag{7}$$

Here, $E_1(t)$ is regularization error. $E_2(t)$ and $E_3(t)$ are truncation errors. From Shannon's sampling theorem [2]

$$f(t) = \sum_{n=-\infty}^{n=+\infty} f(n\Delta) \frac{\sin\left(\frac{\pi}{\Delta}(t - n\Delta)\right)}{\frac{\pi}{\Delta}(t - n\Delta)}, \tag{8}$$

which can be differentiated term by term, the total error can be written as a sum of three components

$$E(t) = \sum_{i=1}^{3} E_i(t). \tag{9}$$

The corresponding error norms satisfy

$$\|E(t)\|_{L^2(R)} \leq \sqrt{3} \sum_{i=1}^{3} \|E_i(t)\|_{L^2(R)}. \tag{10}$$

B. Estimation of $E_1(t)$

Let $\hat{f}(\omega)$ be the Fourier transform of $f(x)$, and $\hat{f}(\omega) = \int_R f(x) \exp(ix\omega) dx$. Since

$$\left[\frac{\sin\left(\frac{\pi}{\Delta}(t - n\Delta)\right)}{\frac{\pi}{\Delta}(t - n\Delta)} \right]\hat{}(\omega) = \Delta \exp(-in\Delta\omega)\chi_{[-\frac{\pi}{\Delta}, \frac{\pi}{\Delta}]}(w) \tag{11}$$

and

$$\left[\exp\left(-\frac{(t - n\Delta)^2}{2\sigma^2}\right) \right]\hat{}(\omega) = \sqrt{2\pi}\sigma \exp(-in\Delta\omega - \frac{\sigma^2\omega^2}{2}), \tag{12}$$

one writes

$$\left[\frac{\sin\left(\frac{\pi}{\Delta}(t - n\Delta)\right)}{\frac{\pi}{\Delta}(t - n\Delta)} \right]\hat{}(\omega) * \left[\exp\left(-\frac{(t - n\Delta)^2}{2\sigma^2}\right) \right]\hat{}(\omega)$$

$$= \int_R \Delta\sqrt{2\pi}\sigma \exp(-in\Delta(\omega - \theta))\chi_{[\theta - \frac{\pi}{\Delta}, \theta + \frac{\pi}{\Delta}]}(\omega) \exp(-in\Delta\theta - \frac{\sigma^2\theta^2}{2}) d\theta$$

$$= \Delta\sqrt{2\pi}\sigma \exp(-in\Delta\omega) \int_{\theta - \frac{\pi}{\Delta}}^{\theta + \frac{\pi}{\Delta}} \exp(-\frac{\sigma^2\theta^2}{2}) d\theta. \tag{13}$$

From Eq. (13)

$$\left[\sum_{n=-\infty}^{n=+\infty} f(n\Delta)\frac{\sin\left(\frac{\pi}{\Delta}(t-n\Delta)\right)}{\frac{\pi}{\Delta}(t-n\Delta)}\exp\left(-\frac{(t-n\Delta)^2}{2\sigma^2}\right)\right]\hat{\,}(\omega)$$

$$=\sum_{n=-\infty}^{n=+\infty} f(n\Delta)\frac{1}{2\pi}\left[\frac{\sin\left(\frac{\pi}{\Delta}(t-n\Delta)\right)}{\frac{\pi}{\Delta}(t-n\Delta)}\hat{]}(\omega)*\left[\exp\left(-\frac{(t-n\Delta)^2}{2\sigma^2}\right)\right]\hat{\,}(\omega)\right.$$

$$=\sum_{n=-\infty}^{n=+\infty} f(n\Delta)\Delta\exp(-in\Delta\omega)\frac{1}{\sqrt{\pi}}\int_{\frac{\sigma(\omega-\frac{\pi}{\Delta})}{\sqrt{2}}}^{\frac{\sigma(\omega+\frac{\pi}{\Delta})}{\sqrt{2}}}\exp(-t^2)dt. \tag{14}$$

Since function f satisfies

$$\hat{f}(\omega)\in L^2[-B,B]\subset L^2[-\frac{\pi}{\Delta},\frac{\pi}{\Delta}], \tag{15}$$

it has a Fourier series expansion

$$\hat{f}(\omega)=\sum_{n=-\infty}^{\infty} c_n\exp(in\Delta\omega), \tag{16}$$

where coefficients is given by

$$c_n=\frac{\Delta}{2\pi}\int_{-\frac{\pi}{\Delta}}^{\frac{\pi}{\Delta}}\hat{f}(\omega)\exp(-in\Delta\omega)d\omega=\Delta f(-n\Delta). \tag{17}$$

Equivalently, $\hat{f}(\omega)$ can be written

$$\hat{f}(\omega)=\hat{f}(\omega)\chi_{[-B,B]}(\omega)=\sum_{n=-\infty}^{\infty}\Delta f(n\Delta)\exp(-in\Delta\omega)\chi_{[-B,B]}(\omega). \tag{18}$$

Denote

$$\varepsilon(\omega)=\chi_{[-B,B]}(\omega)-\frac{1}{\sqrt{\pi}}\int_{\frac{\sigma(\omega-\frac{\pi}{\Delta})}{\sqrt{2}}}^{\frac{\sigma(\omega+\frac{\pi}{\Delta})}{\sqrt{2}}}\exp(-t^2)dt, \tag{19}$$

then combining Eqs. (5), (14), (16) and (18), one has

$$\hat{E_1}(\omega)=(i\omega)^s\hat{f}(\omega)\varepsilon(\omega). \tag{20}$$

For $\omega\in[-B,B]$, $\varepsilon(\omega)$ can be evaluated as

$$\varepsilon(\omega)=\frac{1}{\sqrt{\pi}}\left[\int_{-\infty}^{\infty}\exp(-t^2)dt-\int_{\frac{\sigma(\omega-\frac{\pi}{\Delta})}{\sqrt{2}}}^{\frac{\sigma(\omega+\frac{\pi}{\Delta})}{\sqrt{2}}}\exp(-t^2)dt\right]$$

$$=\frac{1}{\sqrt{\pi}}\left[\int_{\frac{\sigma(\frac{\pi}{\Delta}-\omega)}{\sqrt{2}}}^{\infty}\exp(-t^2)dt+\int_{\frac{\sigma(\omega+\frac{\pi}{\Delta})}{\sqrt{2}}}^{\infty}\exp(-t^2)dt\right]. \tag{21}$$

Moreover, for $x\geq 0$, the following inequality [12] is valid

$$\frac{1}{x+\sqrt{x^2+2}}\leq\exp(x^2)\int_x^{\infty}\exp(-t^2)dt\leq\frac{1}{x+\sqrt{x^2+\frac{4}{\pi}}}. \tag{22}$$

Therefore, the estimation for $\varepsilon(\omega)$ is obtained as

$$\varepsilon(\omega)\leq\frac{1}{\sqrt{\pi}}\left(\frac{\exp\left(-\frac{\sigma^2(\frac{\pi}{\Delta}-\omega)^2}{2}\right)}{\sqrt{2}\sigma(\frac{\pi}{\Delta}-\omega)}+\frac{\exp\left(-\frac{\sigma^2(\frac{\pi}{\Delta}+\omega)^2}{2}\right)}{\sqrt{2}\sigma(\frac{\pi}{\Delta}+\omega)}\right)$$

$$\leq\frac{1}{\sigma(\frac{\pi}{\Delta}-B)\exp\left(\frac{\sigma^2(\frac{\pi}{\Delta}-B)^2}{2}\right)}. \tag{23}$$

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It follows from Eqs. (20) and (23) that

$$E_1\hat{}(\omega) \leq \frac{f\hat{}(\omega)(i\omega)^s}{\sigma(\frac{\pi}{\Delta} - B)\exp(\frac{\sigma^2(\frac{\pi}{\Delta}-B)^2}{2})}. \tag{24}$$

From the Parseval identity, one has

$$\|E_1(t)\|_{L^2(R)} = \frac{1}{2\pi}\|E_1\hat{}(\omega)\|_{L^2(R)}$$

$$\leq \frac{\|f^{(s)}(t)\|_{L^2(R)}}{2\pi\sigma(\frac{\pi}{\Delta} - B)\exp\left(\frac{\sigma^2(\frac{\pi}{\Delta}-B)^2}{2}\right)}. \tag{25}$$

C. Estimation of $E_2(t)$

Differentiations can be written

$$E_2(t) = \sum_{n \geq \lceil \frac{t}{\Delta} \rceil + M_1} f(n\Delta) \left[\sum_{i+j+k=s} \frac{s!}{i!k!}(\frac{\pi}{\Delta})^{i-1}\sin(\frac{\pi}{\Delta}t - n\pi + \frac{\pi i}{2}) \right.$$

$$\left. \frac{(-1)^j}{(t-n\Delta)^{j+1}}\frac{(-1)^k}{(\sqrt{2}\sigma)^k}H_k(\frac{t-n\Delta}{\sqrt{2}\sigma})\exp\left(-\frac{(t-n\Delta)^2}{2\sigma^2}\right)\right], \tag{26}$$

where $H_k(x)$ is the Hermite polynomial

$$\exp(-x^2)H_k(x) = (-1)^k(\frac{d}{dx})^k\exp(-x^2). \tag{27}$$

Let $l = n - \lceil \frac{t}{\Delta} \rceil$, where $\lceil x \rceil$ is the integral part of x and $\lfloor x \rfloor = x - \lceil x \rceil$, then

$$E_2(t) = \sum_{l \geq M_1} f(t + l\Delta - \lfloor \frac{t}{\Delta} \rfloor \Delta) \left[\sum_{i+j+k=s} \frac{s!}{i!k!}(\frac{\pi}{\Delta})^{i-1}(-1)^{j+k+l} \right.$$

$$\sin\left(\lfloor \frac{t}{\Delta} \rfloor \pi + \frac{\pi i}{2}\right) \frac{1}{(\sqrt{2}\sigma)^k \Delta^{j+1}(-l + \lfloor \frac{t}{\Delta} \rfloor)^{j+1}}$$

$$\left[H_k\left(\frac{-l\Delta + \lfloor \frac{t}{\Delta} \rfloor \Delta}{\sqrt{2}\sigma}\right)\right] \exp\left(-\frac{(l\Delta - \lfloor \frac{t}{\Delta} \rfloor \Delta)^2}{2\sigma^2}\right)$$

$$= \sum_{i+j+k=s}\sum_{l \geq M_1} F_k(l)s_{i,j,k}(l), \tag{28}$$

where

$$F_k(l) = f(t + l\Delta - \lfloor \frac{t}{\Delta} \rfloor \Delta)H_k\left(\frac{-l\Delta + \lfloor \frac{t}{\Delta} \rfloor \Delta}{\sqrt{2}\sigma}\right)$$

$$\exp\left(-\frac{(l\Delta - \lfloor \frac{t}{\Delta} \rfloor \Delta)^2}{2\sigma^2}\right) \tag{29}$$

$$s_{i,j,k}(l) = (-1)^l \frac{s!\pi^{i-1}(-1)^{j+k}\sin(\lfloor \frac{t}{\Delta} \rfloor \pi + \frac{\pi i}{2})}{i!k!\Delta^{i+j}(-l + \lfloor \frac{t}{\Delta} \rfloor)^{j+1}(\sqrt{2}\sigma)^k}. \tag{30}$$

Two simple lemmas are required.

Lemma 1 (Abel's inequality) [13]. For two sequences $\{a_n\}, \{b_n\}, b_1 \geq b_2 \geq \ldots \geq b_n, a_n, b_n \in R$, set

$$s_k = \sum_{i=1}^{k} a_i \tag{31}$$

$$m = \min_{1 \le k \le n} s_k \tag{32}$$

$$M = \max_{1 \le k \le n} s_k, \tag{33}$$

then

$$mb_1 \le \sum_{i=1}^{n} a_i b_i \le Mb_1. \tag{34}$$

Lemma 2. As all the notations unchanged, set $g(x) = f(x)H_k(\frac{t-x}{\sqrt{2}\sigma})$. If $g(x)$ satisfies

$$g'(x) \le g(x)\frac{(x-t)}{\sigma^2}, \tag{35}$$

whenever $x \ge t + (M_1 - 1)\Delta$, then $\{F_k(l)\}_{l \in \mathcal{N}}$ is a decreasing sequence.

The proof is obvious by taking the first order derivative.

Let denote

$$S_{i,j,k}(N) = \sum_{l \ge M_1}^{M_1+N} s_{i,j,k}(l). \tag{36}$$

It is estimated that

$$
\begin{aligned}
|S_{i,j,k}(N)| &= \left| \sum_{l \ge M_1}^{M_1+N} (-1)^l \frac{s!\pi^{i-1}\sin(\lfloor\frac{t}{\Delta}\rfloor\pi + \frac{\pi i}{2})(-1)^{k+j}}{i!k!\Delta^{i+j}(\sqrt{2}\sigma)^k} \frac{1}{(-l+\lfloor\frac{t}{\Delta}\rfloor)^{j+1}} \right| \\
&= \left| \frac{s!\pi^{i-1}\sin(\lfloor\frac{t}{\Delta}\rfloor\pi + \frac{\pi i}{2})(-1)^{k+j}}{i!k!\Delta^{i+j}(\sqrt{2}\sigma)^k} \sum_{l \ge M_1}^{M_1+N} (-1)^l \frac{1}{(-l+\lfloor\frac{t}{\Delta}\rfloor)^{j+1}} \right| \\
&\le \frac{s!\pi^{i-1}}{i!k!\Delta^{i+j}(\sqrt{2}\sigma)^k} \frac{1}{(M_1-1)^{j+1}}.
\end{aligned} \tag{37}
$$

Then from (28) and (37), and by using lemma 1 and lemma 2, one has

$$
\begin{aligned}
E_2(t) &\le f(t + M_1\Delta)\exp\left(-\frac{(M_1\Delta)^2}{2\sigma^2}\right) \\
&\times \sum_{i+j+k=s} \frac{s!\pi^{i-1}H_k(\frac{-M_1\Delta}{\sqrt{2}\sigma})}{i!k!\Delta^{i-1}(\sqrt{2}\sigma)^k((M_1-1)\Delta)^{j+1}}.
\end{aligned} \tag{38}
$$

This gives rise to

$$\|E_2(t)\|_{L^2(R)} \le \frac{\|f(t)\|_{L^2(R)} \sum_{i+j+k=s} \frac{s!\pi^{i-1}H_k(\frac{-M_1\Delta}{\sqrt{2}\sigma})}{i!k!\Delta^{i-1}(\sqrt{2}\sigma)^k((M_1-1)\Delta)^{j+1}}}{\exp\left(\frac{(M_1\Delta)^2}{2\sigma^2}\right)}. \tag{39}$$

D. Estimation of $E_3(t)$

A result like lemma 2 is required.

Lemma 3. Notations are the same as before. Denote $g(x) = f(x)H_k(\frac{t-x}{\sqrt{2}\sigma})$, if $g(x)$ satisfies

$$g'(x) \ge g(x)\frac{(x-t)}{\sigma^2}, \tag{40}$$

whenever $x \leq t - M_2\Delta$, then $\{F_k(l)\}_{l \in \mathcal{N}}$ is an increasing sequence.

The proof is also direct. Therefore, by the same treatment as that in the previous subsection, we obtain

$$\|E_3(t)\|_{L^2(R)} \leq \frac{\|f(t)\|_{L^2(R)} \sum_{i+j+k=s} \frac{s!\pi^{i-1}H_k(\frac{-M_2\Delta}{\sqrt{2}\sigma})}{i!k!\Delta^{i-1}(\sqrt{2}\sigma)^k(M_2\Delta)^{j+1}}}{\exp\left(\frac{(M_2\Delta)^2}{2\sigma^2}\right)}. \tag{41}$$

E. The end of the proof

By combining Eqs. (10), (25), (39) and (41), one obtains Eq. (3).

IV. DISCUSSION

Remark 1. For $s = 0$, one has

$$\|f(t) - \sum_{n=\lceil\frac{t}{\Delta}\rceil-M_2}^{\lceil\frac{t}{\Delta}\rceil+M_1} f(n\Delta)\frac{\sin\left(\frac{\pi}{\Delta}(t-n\Delta)\right)}{\frac{\pi}{\Delta}(t-n\Delta)}\exp\left(-\frac{(t-n\Delta)^2}{2\sigma^2}\right)\|_{L^2(R)}$$

$$\leq \sqrt{3}\|f(t)\|_{L^2(R)} \left\{ \frac{1}{2\pi\sigma(\frac{\pi}{\Delta}-B)\exp\left(\frac{\sigma^2(\frac{\pi}{\Delta}-B)^2}{2}\right)} \right.$$

$$\left. + \frac{1}{(M_1-1)\pi\exp\left(\frac{(M_1\Delta)^2}{2\sigma^2}\right)} + \frac{1}{M_2\pi\exp\left(\frac{(M_2\Delta)^2}{2\sigma^2}\right)} \right\}. \tag{42}$$

This is a rigorous error statement for the formulae widely used in the aforementioned numerical computations. Roughly speaking, if $\exp(-\frac{x^2}{2}) = 10^{-\eta}$, then $\eta = \frac{x^2}{2ln10}$, so the error is

$$\varepsilon(r, B, \Delta, M) = \sqrt{3}\|f(t)\|_{L^2(R)} \left(\frac{1}{2\pi r(\pi - B\Delta)10^{\frac{r^2(\pi-B\Delta)^2}{2ln10}}} \right.$$

$$\left. + \frac{1}{(M_1-1)\Delta 10^{\frac{(M_1-1)^2}{2r^2 ln10}}} + \frac{1}{M_2\Delta 10^{\frac{(M_2)^2}{2r^2 ln10}}} \right), \tag{43}$$

where $r = \frac{\sigma}{\Delta}$. One may choose r, B, Δ and M appropriately to attain desired accuracy. Assume all non-exponential quantities are combined to give unit, and $M = M_1 - 1 = M_2$, one has

$$r(\pi - B\Delta) > \sqrt{\eta 2 \ln 10} \tag{44}$$

and

$$\frac{M}{r} > \sqrt{\eta 2 \ln 10}, \tag{45}$$

where η is the desired order of accuracy. There are some general rules for attaining high accuracy. These are discussed from two different arguments.

1.) For a given function $f(x)$ with a known bandlimit B, other parameters, Δ, r and M, are to be chosen appropriately to achieve a desired accuracy order η:

(i) From Eqs. (44) and (45) one has $B\Delta \leq \pi - \frac{\sqrt{\eta 2 \ln 10}}{r}$. For fixed r, the higher the frequency bandlimit B is, the smaller Δ should be, which means the more grid points in the computational domain. When Δ varies from 0 to $\frac{\pi}{B}$, r changes from $\frac{\sqrt{\eta 2 \ln 10}}{\pi}$ to $+\infty$, therefore for sufficiently small Δ, r is near $\frac{\sqrt{\eta 2 \ln 10}}{\pi}$.

(ii) No matter how many grid points are in the computational domain, r and M cannot be too small. Equations (44) and (45) indicate $r > \frac{\sqrt{\eta 2 \ln 10}}{\pi}$ and $M > r\sqrt{\eta 2 \ln 10}$. If M and r are less than the minimal requirements, the

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accuracy deteriorates quickly. On the other hand, if sufficiently large r and M are used, say, $M = 30$ and $r = 3.5$, high approximation accuracy can be achieved.

2.) In practical computations, such as in solving a partial differential equation, the function f and its B are unknown. In this case, Δ is selected a priori. Then r and M are to be chosen properly for achieving a desired accuracy order η:

(i) For a given grid spacing, Δ, and accuracy requirement η, r value determines frequency bandlimit B which can be reached. Then the set of functions f which are almost bandlimited to B can be accurately approximated (where 'almost bandlimited to B' means the function f is not necessarily bandlimited but its Fourier amplitude outside $|B|$ is much smaller than the given error $10^{-\eta}$). The choice of M should be consistent with r for a given accuracy requirement. In general, small r and M values lead to an accurate approximation for low frequency component of a function of interest. But the prediction of a high frequency component will not be accurate in such a case.

(ii) For a given grid spacing Δ and r value, the larger M is, the higher bandlimit B can be reached.

(iii) To improve computational efficiency with a given Δ, B shall be very close to $\frac{\pi}{\Delta}$. However, to maintain certain approximation accuracy, r has to be sufficiently large, which implies that M has to be very large too. This in turn results in low efficiency (It takes $M \to \infty$ to maintain the accuracy if one samples at the Nyquist rate).

(iv) If Δ, M and η are chosen, then r is also fixed. For example, to achieve the machine precision $10^{-\eta} \sim 10^{-15}$, Eq. (44) estimates $r > 2.8$. If this is achieved by using $M = 33$, then Eq. (45) estimates $r < 4$. In fact, $M \sim 30$ and $2.8 < r < 4.0$ are the parameter regions found from an earlier numerical test [6] and were used in many applications [7–11].

Remark 2. A comparison between the truncation errors of Shannon's sampling formulae and the regularized Shannon's sampling formulae is in order. Reference [4] estimates that the expression

$$(T_N f)(t) = f(t) - \sum_{n=-N}^{n=+N} f(n\Delta) \frac{\sin(\frac{\pi}{\Delta}(t - n\Delta))}{\frac{\pi}{\Delta}(t - n\Delta)} \tag{46}$$

has error of

$$|T_N(t)| \leq \frac{\sqrt{2}}{\pi} \sqrt{E} \left| \sin(\frac{\pi t}{\Delta}) \right| \sqrt{\frac{N\Delta}{(N\Delta^2 - t^2)}}, \tag{47}$$

where $t < N\Delta$, and E is the total 'energy' of the function given by

$$E = \int_{-\frac{\pi}{\Delta}}^{\frac{\pi}{\Delta}} |\hat{f}(w)|^2 dw. \tag{48}$$

This is not *directly* comparable with our error estimate because our sampling is centered around a point of interest, x. Let consider a truncation error of the form

$$(E_M f)(t) = f(t) - \sum_{n=\lceil \frac{t}{\Delta} \rceil - M}^{n=\lceil \frac{t}{\Delta} \rceil + M} f(n\Delta) \frac{\sin(\frac{\pi}{\Delta}(t - n\Delta))}{\frac{\pi}{\Delta}(t - n\Delta)}. \tag{49}$$

In Appendix A, it is shown that in a finite computational domain, the L^2 norm of $(E_M f)(t)$ has the order of $\|f(t)\|_{L^2(R)} \sqrt{\frac{1}{M\Delta}}$, which is much larger than the truncation error of the regularized Shannon's formulae. On the other hand, to achieve the same accuracy, the regularized formulae requires much fewer computational grids [1,6].

Remark 3. Discussions for the higher order derivatives can be presented in a similar manner as those of Remarks 1 and 2. In fact, previous work of solving partial differential equations [1,6–11]. involved such derivatives, and results are consistent with the present theorem. Detailed comparison is omitted.

Remark 4. In many practical applications, such as in solving partial differential equations, error estimations and discussions in other spaces are often required. Moreover, in real computations, the computational domain is always limited to a finite interval, such as $[a, b]$. Therefore, the norm $\|f\|_{L^2(R)}$ in Eqs. (39) and (41) are required to be changed into $\|f\|_{L^2(a,b)}$, which can be evaluated by integrations along $[a + M_1\Delta, b + M_1\Delta]$ and $[a - M_2\Delta, b - M_2\Delta]$ respectively. Therefore various $L^p(1 \leq p \leq 2)$ error estimates of $E(t)$ can be derived accordingly. If we know the size of L^p norm $(1 \leq p \leq 2)$ of the function of interest, then we can deduce from the theorem the critical values, r and M, to achieve desired accuracy.

[1] G. W. Wei, "Discrete singular convolution for the solution of the Fokker-Planck equation", *J. Chem. Phys.*, vol. 110, 8930-8942 (1999).

[2] C. E. Shannon, "A mathematical theory of communication", *Bell System Tech. J.,* 27, 379-423 (1948).

[3] Charles K. Chui, *An Introduction to Wavelets*, Academic Press, 1992.

[4] Robert J. Marks II, *Introduction to Shannon Sampling and Interpolation Theory*, Spring-Verlag, 1991.

[5] G. W. Wei, D. S. Zhang, D. J. Kouri and D. K. Hoffman, "Lagrange Distributed Approximating Functionals", *Phys. Rev. Lett.*, vol. 79, 775-779 (1997).

[6] G. W. Wei, "Quasi wavelets and quasi interpolating wavelets", *Chem. Phys. Lett.*, vol. 296, 215-222 (1998).

[7] G. W. Wei, "Discrete singular convolution method for the Sine-Gordon equation", *Physica* D, vol. 137, 247-259 (2000).

[8] G. W. Wei "A unified computational method for solving mechanical problems", *Commun. Numer. Methods Engng.*, submitted; D. C. Wan and G. W. Wei, "Numerical solution of unsteady incompressible flows by the discrete singular convolution", *Int. J. Numer. Methods Fluid*, submitted.

[9] G. W. Wei and Y. Gu, "A novel approach for Burgers' equation with high Reynolds number", unpublished.

[10] G. W. Wei, "Solving quantum eigenvalue problems by discrete singular convolution", *J. Phys. B*, vol. 33, 343-352 (2000).

[11] S. Guan, C.-H. Lai and G. W. Wei, "Boundary Controlled Nanoscale Morphology in a Circular Domain", *Physica D*, submitted.

[12] D. Zwillinger, *Handbook of Integration*, Jones and Barlett, 1992.

[13] D. S. Mitrinovic, *Analytic Inequalities*, Spring-Verlag, 1970.

APPENDIX A: TRUNCATION ERROR OF SHANNON'S SAMPLING FORMULAE

Lemma 4. In the computational domain $[a, b]$, the error expression

$$(E_M f)(t) = f(t) - \sum_{n=\lceil \frac{t}{\Delta} \rceil - M}^{n=\lceil \frac{t}{\Delta} \rceil + M} f(n\Delta) \frac{\sin(\frac{\pi}{\Delta}(t - n\Delta))}{\frac{\pi}{\Delta}(t - n\Delta)} \tag{A1}$$

satisfies the estimate

$$\|(E_M f)(t)\|_{L^2(a,b)} \leq \frac{2\|f(t)\|_{L^2(R)}}{\sqrt{(M-2)\Delta}}. \tag{A2}$$

Proof. Let denote

$$f_M(t) = \frac{1}{\pi} \sin\left(\frac{\pi t}{\Delta}\right) \sum_{n=\lceil \frac{t}{\Delta} \rceil - M}^{n=\lceil \frac{t}{\Delta} \rceil + M} \frac{f(n\Delta)(-1)^n}{(\frac{t}{\Delta} - n)}. \tag{A3}$$

By using Schwartz's inequality, one has

$$\left(\sum_{n=\lceil \frac{t}{\Delta} \rceil + M}^{n=+\infty} \frac{f(n\Delta)(-1)^n}{(\frac{t}{\Delta} - n)} \right)^2$$

$$\leq \|f(t)\|_{L^2(R)}^2 \sum_{n=\lceil \frac{t}{\Delta} \rceil + M}^{n=+\infty} \frac{1}{(t - n\Delta)^2}$$

$$\leq \frac{1}{\Delta^2} \|f(t)\|_{L^2(R)}^2 \sum_{l \geq M} \frac{1}{(l-1)^2}$$

$$\leq \frac{1}{\Delta^2} \|f(t)\|_{L^2(R)}^2 \int_{M-2}^{+\infty} \frac{dx}{x^2}$$

$$= \frac{\|f(t)\|_{L^2(R)}^2}{(M-2)\Delta^2}. \tag{A4}$$

Similarly one obtains

$$\left(\sum_{n=-\infty}^{n=\lceil \frac{t}{\Delta} \rceil -M} \frac{f(n\Delta)(-1)^n}{(\frac{t}{\Delta}-n)}\right)^2 \leq \frac{\|f(t)\|_{L^2(R)}^2}{(M-1)\Delta^2}. \tag{A5}$$

By combining Eqs. (A3), (A4) and (A5), one finishes the proof.